

Spin-wave series for quantum one-dimensional ferrimagnets

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Abstract

Second-order spin-wave expansions are used to compute the ground-state energy and sublattice magnetizations of the quantum one-dimensional Heisenberg ferrimagnet with nearest-neighbor antiferromagnetic interactions and two types of alternating sublattice spins $S_1 > S_2$. It is found that in the extreme quantum cases $(S_1, S_2) = (1, 1/2)$, $(3/2, 1)$, and $(3/2, 1/2)$, the estimates for the ground-state energy and sublattice magnetizations differ less than 0.03% for the energy and 0.2% for the sublattice magnetizations from the recently published density matrix renormalization group numerical calculations. The reported results strongly suggest that the quantum Heisenberg ferrimagnetic chains give another example of a low-dimensional quantum spin system where the spin-wave approach demonstrates a surprising efficiency.

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Recently, two scientific groups have published theoretical results concerning the model of the one-dimensional Heisenberg ferrimagnet (1DQHF) containing two alternating site spins ($S_1 > S_2$) per unitary cell and nearest-neighbor antiferromagnetic bonds [1–4]. The presented linear spin-wave analysis demonstrates a substantial reduction of the classical sublattice spins imposed by the quantum fluctuations. In the extreme quantum cases with $(S_1, S_2) = (1, 1/2)$, $(3/2, 1)$, and $(3/2, 1/2)$, the quantum reduction of S_2 was shown to be about 61%, 46%, and 37%, respectively. The density matrix renormalization group results [4] point towards a smaller reduction. The cited values are respectively reduced to 42%, 36%, and 28%. For comparison, in the square-lattice Heisenberg antiferromagnet the discussed reduction is about 39%. It is clear that the linear theory overestimates the role of the zero-point spin fluctuations. In this respect, an open question is if the qualitative picture based on the LSWT (and concerning, in particular, the structure of the elementary excitations) can reflect the real situation at all. The purpose of the present paper is to throw some light on the above problem through an explicit study of the large S series for the ground state energy and sublattice magnetizations up to second order in $1/S$.

The Hamiltonian of the 1DQHF with two spins $S_1 > S_2$ per unitary cell and nearest-neighbor antiferromagnetic couplings reads

$$H = \sum_{n,\delta} \mathbf{S}_{1n} \mathbf{S}_{2n+\delta}, \quad (1)$$

where the intergers n number the cells and the vector $\delta = \pm 1/2$ connects the two nearest-neighbor spins. The size of the elementary cell and the exchange interaction are unities. In what follows we frequently use the notations $S_1/S_2 \equiv w$, $S_2 \equiv S$.

We will use the Dyson-Maleev representation for the site spin operators. After some standard procedures [5], including the Fourier and Bogoliubov transformations and the normal ordering of the boson operators, the spin Hamiltonian can be recasted to the following form

$$H = H_0 + V, \quad V = c_1 + V_2 + V_{DM}, \quad (2)$$

$$H_0 = \left(-2wS^2 + 2Sc_0\right)N + 2S \sum_k \left[\omega_k^{(\alpha)} \alpha_k^\dagger \alpha_k + \omega_k^{(\beta)} \beta_k^\dagger \beta_k\right], \quad (3)$$

$$V_2 = \sum_k \left[V_k^{(1)} \alpha_k^\dagger \alpha_k + V_k^{(2)} \beta_k^\dagger \beta_k + V_k^{(3)} \alpha_k^\dagger \beta_k^\dagger + V_k^{(4)} \alpha_k \beta_k\right], \quad (4)$$

where $c_0 = -[1 - (1/N) \sum_k \epsilon_k](w + 1)/2$, $c_1 = -2(g_1^2 + g_2^2) - 2g_1g_2(w + 1)w^{-1/2}$, $g_1 = -(1/2N) \sum_k \gamma_k \eta_k / \epsilon_k$, $g_2 = -(1/2) + (1/2N) \sum_k 1/\epsilon_k$, $\epsilon_k = (1 - \eta_k^2)^{1/2}$, $\eta_k = 2\gamma_k w^{1/2}/(w + 1)$, $\gamma_k = \cos(k/2)$, and N is the number of cells.

H_0 is the quadratic LSWT Hamiltonian. The boson operators α_k and β_k describe two types of elementary excitations with energies

$$E_k^{(\alpha, \beta)} = 2S\omega_k^{(\alpha, \beta)} = 2S \left[\frac{w+1}{2} \epsilon_k \mp \frac{(w-1)}{2} \right]. \quad (5)$$

The α excitations are gapless ($\omega_k^{(\alpha)} \sim k^2$ for small k) and describe magnons in the sector with a total spin $(S_1 - S_2)N - 1$, whereas the β excitations are gapful ($\omega_k^{(\beta)} = w - 1 + O(k^2)$) and belong to the sector $(S_1 - S_2)N + 1$.

The interaction V contains three different terms: The constant c_1 gives the first-order correction to the ground state energy. The quadratic interaction V_2 introduces four vertex functions defined as follows

$$V_k^{(1)} = -\frac{g_1}{\epsilon_k} \left(\frac{w+1}{\sqrt{w}} - 2\gamma_k \eta_k + \frac{w-1}{\sqrt{w}} \epsilon_k \right) - \frac{g_2}{\epsilon_k} \left(2 - \frac{w+1}{\sqrt{w}} \gamma_k \eta_k \right) \quad (6)$$

$$V_k^{(3)} = -\frac{g_1}{\epsilon_k} \left(2\gamma_k - \frac{w+1}{\sqrt{w}} \eta_k \right) - \frac{g_2}{\epsilon_k} \left(\frac{w+1}{\sqrt{w}} \gamma_k + \frac{w-1}{\sqrt{w}} \gamma_k \epsilon_k - 2\eta_k \right) \quad (7)$$

$$V_k^{(4)} = V_k^{(3)} + 2g_2 \frac{w-1}{\sqrt{w}} \gamma_k, \quad V_k^{(2)} = V_k^{(1)} - 2g_1 \frac{w-1}{\sqrt{w}}. \quad (8)$$

For the model under consideration the off-diagonal terms of V_2 do not vanish due to the inequality $S_1 > S_2$. Note also that V_2 is a non-Hermitian operator for the same reason.

V_{DM} is the Dyson-Maleev normal ordered quartic interaction, containing nine vertex functions $V^{(i)} = V_{12,34}^{(i)}$, $i = 1, \dots, 9$. We have adopted the symmetric form used in Refs. [6,7] and the convention $(k_1, k_2, k_3, k_4) \equiv (1, 2, 3, 4)$.

Now, let us represent the series for the ground state energy and the magnetization of the first sublattice in the following form

$$\frac{E_0}{N} = -2wS^2 + 2Sc_0 + c_1 + \frac{c_2}{2S} + \dots, \quad (9)$$

$$m_1 = wS + b_0 + \frac{b_1}{2S} + \frac{b_2}{(2S)^2} + \dots \quad (10)$$

The coefficient $b_0 = -g_2$ gives the spin reduction in the LSWT. The first-order correction for m_1 is related to the off-diagonal terms in V_2 , and a simple calculation gives the following result

$$b_1 = -\frac{1}{2(w+1)} \frac{1}{N} \sum_k (V_k^{(3)} + V_k^{(4)}) \frac{\eta_k}{\epsilon_k^2}. \quad (11)$$

The coefficients c_2 and b_2 will be calculated using the Rayleigh-Schrodinger perturbation theory. A straightforward calculation gives the following two contributions to $c_2 = c_{21} + c_{22}$ resulting from V_2 and V_{DM} , respectively

$$c_{21} = -\frac{1}{w+1} \frac{1}{N} \sum_k \frac{V_k^{(3)} V_k^{(4)}}{\epsilon_k}, \quad c_{22} = -\frac{2}{w+1} \frac{1}{N^3} \sum_{1-4} \delta_{12}^{34} \frac{V_{12;34}^{(7)} V_{34;12}^{(8)}}{\epsilon_1 + \epsilon_2 + \epsilon_3 + \epsilon_4}. \quad (12)$$

. Here δ_{12}^{34} is the Kronicker function. The symmetric vertex functions $V_{12;34}^{(7)}$ and $V_{12;34}^{(8)}$ read

$$V_{12;34}^{(7)} = \mathcal{U}_{1234} \left\{ x_1 \left[x_4 (\gamma_{1-3} - w^{-1/2} x_3 \gamma_1) - (w^{1/2} \gamma_{1-3-4} - x_3 \gamma_{1-4}) \right] \right. \\ \left. + x_2 \left[x_4 (\gamma_{2-3} - w^{-1/2} x_3 \gamma_2) - (w^{1/2} \gamma_{2-3-4} - x_3 \gamma_{2-4}) \right] \right\}, \quad (13)$$

$$V_{12;34}^{(8)} = \mathcal{U}_{1234} \left\{ x_2 \left[(x_3 \gamma_{1-3} - w^{-1/2} \gamma_1) - x_4 (w^{1/2} x_3 \gamma_{1-3-4} - \gamma_{1-4}) \right] \right. \\ \left. + x_1 \left[(x_3 \gamma_{2-3} - w^{-1/2} \gamma_2) - x_4 (w^{1/2} x_3 \gamma_{2-3-4} - \gamma_{2-4}) \right] \right\}, \quad (14)$$

where $\mathcal{U}_{1234} = u_1 u_2 u_3 u_4$, $u_k = (1 + \epsilon_k)/2\epsilon_k$, and $x_k = \eta_k/(1 + \epsilon_k)$.

To calculate b_2 we introduce in H a staggered magnetic field for S_1 spins through the operator $-h_1 \sum_n S_{1n}^z$. Then the required second-order correction for m_1 can be deduced from $m_1^{(2)} = -(1/N)[\partial E_0^{(2)}(h_1)/\partial h_1]|_{h_1=0}$, where $E_0^{(2)}(h_1)$ is the second-order correction to E_0 in a finite h_1 . As a matter of fact, h_1 reduces the structure factor to $\eta_k \mapsto \eta_k =$

$2\gamma_k w^{1/2}/(1+w+h_1/2S)$, and this is all one needs to find all necessary derivatives. In some cases, it is better to use an infinitesimal perturbing field h_1 and the related perturbed ground state $|0_{h_1}\rangle = |0\rangle + [h_1/2S(w+1)] \sum_k (\eta_k/\epsilon_k^2) \alpha_k^\dagger \beta_k^\dagger |0\rangle + O(h_1^2)$.

Using the latter approach, one can easily find [7] two of the contributions to $b_2 = b_{21} + b_{22} + b_{23} + b_{24}$ related to the interaction V_{DM}

$$b_{21} = -\frac{2}{(w+1)^2} \frac{1}{N^3} \sum_{1-4} \delta_{12}^{34} \frac{V_{12;34}^{(7)} V_{34;12}^{(8)}}{(\epsilon_1 + \epsilon_2 + \epsilon_3 + \epsilon_4)^2} \left(\frac{1}{\epsilon_1} + \frac{1}{\epsilon_2} + \frac{1}{\epsilon_3} + \frac{1}{\epsilon_4} \right), \quad (15)$$

$$b_{22} = \frac{2w^{1/2}}{(w+1)^3} \frac{1}{N^3} \sum_{1-4} \delta_{12}^{34} \frac{W_{12;34}}{\epsilon_1 + \epsilon_2 + \epsilon_3 + \epsilon_4}, \quad (16)$$

$$W_{12;34} = V_{12;34}^{(7)} \left[\frac{\gamma_2}{\epsilon_2^2} V_{34;12}^{(5)} + \frac{\gamma_3}{\epsilon_3^2} V_{34;12}^{(2)} \right] + \left[\frac{\gamma_1}{\epsilon_1^2} V_{12;34}^{(6)} + \frac{\gamma_4}{\epsilon_4^2} V_{12;34}^{(3)} \right] V_{34;12}^{(8)}. \quad (17)$$

The vertex functions appearing in the last equation have the same structure as $V_{12;34}^{(7)}$ and $V_{12;34}^{(8)}$ and we will not present here their explicit expressions.

For the other two contributions to b_2 , which are related to the interaction V_2 , we use the first of the mentioned methods. The result reads

$$b_{23} = -\frac{1}{(w+1)^2} \frac{1}{N} \sum_k \frac{V_k^{(3)} V_k^{(4)}}{\epsilon_k^3}, \quad b_{24} = \frac{1}{(w+1)^2} \frac{1}{N} \sum_k \frac{1}{\epsilon_k} \left[U_k^{(3)} V_k^{(4)} + U_k^{(4)} V_k^{(3)} \right], \quad (18)$$

where $U_k^{(3)} = -2g_1\gamma_k/\epsilon_k - 2g_2(1-\gamma_k^2)\eta_k/\epsilon_k^3 - g_3[(w+1)w^{-1/2}\gamma_k + (w-1)w^{-1/2}\gamma_k\epsilon_k - 2\eta_k]/\epsilon_k$, $U_k^{(4)} = U_k^{(3)} + 2g_3(w-1)w^{-1/2}\gamma_k$, $g_3 = -(1/2N) \sum_k \eta_k^2/\epsilon_k^3$. Notice that the equation $m_1 + m_2 = S_1 - S_2$, which is connected to the conservation law for the total magnetization, is fulfilled order by order in the spin-wave series, so that it is enough to know only the corrections for one of the sublattice magnetizations.

The results for the series for a number of combinations (S_1, S_2) are presented in the tables. Surprisingly, even in the extreme quantum cases $(3/2, 1)$ and $(1, 1/2)$, the deviations from the density matrix renormalization group results are less than 0.033% for the energy and 0.2% for the sublattice magnetizations. One can also notice that the increase of the ratio $w = S_1/S_2$ for fixed $S_2 \equiv S = 1/2$ leads to a rapid improvement of the series. This

tendency is expected because for large w the quasiclassical spins on the first sublattice act as an effective field on the $S_2 = 1/2$ spins.

It is instructive to compare the series for 1DQHF with those for the square-lattice Heisenberg antiferromagnet (2DQHA) [8]. Let us take the series for $w = 2$ and for the second sublattice magnetization m_2 .

$$\begin{aligned}
1DQHF : \quad \frac{E_0}{N} &= -4S^2 - 0.436456 \times (2S) - 0.024384 + 0.006518 \times \frac{1}{2S} + \dots \\
2DQHA : \quad \frac{E_0}{N} &= -4S^2 - 0.315895 \times (2S) - 0.024948 + 0.000866 \times \frac{1}{2S} + \dots \\
1DQHF : \quad -m_2 &= S - 0.3048865 + 0.1212303 \times \frac{1}{2S} - 0.0224602 \times \frac{1}{(2S)^2} + \dots \\
2DQHA : \quad m &= S - 0.1966019 + 0 \times \frac{1}{2S} + 0.00348 \times \frac{1}{(2S)^2} + \dots
\end{aligned} \tag{19}$$

The E_0 spin-wave series for the compared models have similar structures.. The $1/S$ correction in 1DQHF is somewhat larger, but note that the LSWT reduction is also larger for the 1D model. The values of the coefficients c_1 are very close to each other. As to the sublattice magnetizations, the main difference comes from the lack of b_1 corrections in the 2DQHA which is connected with the symmetry of the square lattice. Note that up to the first order the quantum spin reductions in the models are approximately one and the same. As a whole, the spin-wave series for the 1DQHF demonstrate features which are compatible with those of the 2DQHA spin-wave series. It is well-known that the spin-wave results for the ground state parameters of the $S = 1/2$ square-lattice Heisenberg antiferromagnet are close to the most precise numerical estimates [9]. The reported results strongly suggest that the quantum Heisenberg ferrimagnetic chains give another example of a low-dimensional quantum spin system where the spin-wave approach demonstrates a surprising efficiency.

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TABLES

TABLE I. The coefficients of the spin-wave series for the ground state energy per cell $\epsilon_0 = E_0/N$ of ferrimagnetic chains with two different spins: $S_1 = wS_2$, $S_2 \equiv S$, $w > 1$; $\epsilon_0 = -2wS^2 + c_0(w) \times (2S) + c_1(w) + c_2(w) \times (2S)^{-1} + O[(2S)^{-2}]$

(S_1, S_2)	$w = S_1/S_2$	$c_0(w)$	$c_1(w)$	$c_2(w)$	ϵ_0 (SWT)	ϵ_0 (DMRG) [4]
$(\frac{3}{2}, 1)$	1.5	-0.41403688(9)	-0.03950436(9)	0.00874156(4)	-3.86320737	-3.86192
$(1, \frac{1}{2})$	2	-0.43645559(0)	-0.02438442(5)	0.00651791(7)	-1.45432210	-1.45408
$(\frac{3}{2}, \frac{1}{2})$	3	-0.45803557(4)	-0.01179278(6)	0.00283359(4)	-1.96699477	-1.96724
$(2, \frac{1}{2})$	4	-0.46862597(4)	-0.00691029(8)	0.00139788(3)	-2.47413839	
$(9, \frac{1}{2})$	18	-0.49305421(4)	-0.00037529(8)	0.00002099(5)	-9.49340852	

TABLE II. The coefficients of the spin-wave series for the sublattice magnetization m_1 of ferrimagnetic chains with two different spins: $S_1 = wS_2$, $S_2 \equiv S$, $w > 1$; $m_1 = wS + b_0(w) + b_1(w) \times (2S)^{-1} + b_2(w) \times (2S)^{-2} + O[(2S)^{-3}]$

(S_1, S_2)	$w = S_1/S_2$	$b_0(w)$	$b_1(w)$	$b_2(w)$	m_1 (SWT)	m_1 (DMRG) [4]
$(\frac{3}{2}, 1)$	1.5	-0.46005842(4)	0.22694904(9)	-0.02899689(7)	1.14616688	1.14427
$(1, \frac{1}{2})$	2	-0.30488650(5)	0.12123033(0)	-0.02246016(3)	0.79388366	0.79248
$(\frac{3}{2}, \frac{1}{2})$	3	-0.18644025(0)	0.05316804(7)	-0.01006592(1)	1.35666188	1.35742
$(2, \frac{1}{2})$	4	-0.13512460(0)	0.03000271(9)	-0.00504066(8)	1.88983745	
$(9, \frac{1}{2})$	18	-0.02818572(2)	0.00152353(6)	-0.00007830(4)	8.97325951	